Anisotropic scaling and generalized conformal invariance at Lifshitz points

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The behaviour of the $3D$ axial next-nearest neighbour Ising (ANNNI) model at the uniaxial Lifshitz point is studied using Monte Carlo techniques. A new variant of the Wolff cluster algorithm permits the analysis of systems far larger than in previous studies. The Lifshitz point critical exponents are $\alpha = 0.18(2)$, $\beta = 0.238(5)$ and $\gamma = 1.36(3)$. Data for the spin-spin correlation function are shown to be consistent with the explicit scaling function derived from the assumption of local scale invariance, which is a generalization of conformal invariance to the anisotropic scaling *at* the Lifshitz point.

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The modern understanding of critical phenomena is governed by the notion of scale invariance.[1] For isotropic critical systems the extension from global, spatially homogeneous scaling to space-dependent rescaling factors leads to the requirement of conformal invariance of the correlators. This approach has proven to be very fruitful when examining isotropic equilibrium critical systems, especially in two dimensions.[1–3]

On the other hand, little is known for systems with strongly anisotropic critical points, where the value of the anisotropy exponent θ differs from unity. In these cases, the two-point function $C(\vec{r}_\perp, r_{||})$ satisfies the scaling form

$$C(\vec{r}_\perp, r_{||}) = b^{-2x} C(b\vec{r}_\perp, b^\theta r_{||}) = r_\perp^{-2x}\, \Omega(r_{||} r_\perp^{-\theta}) \qquad (1)$$

where $r_{||}$ and $r_\perp = |\vec{r}_\perp|$ are the distances parallel and perpendicular with respect to a chosen axis, x is a scaling dimension, θ is the anisotropy exponent and $\Omega(v)$ is a scaling function. Scale invariance alone is not enough to determine the form of the function $\Omega(v)$.

Recently, a generalization of conformal invariance involving local space-time-dependent scale transformations for anisotropy exponents $\theta \neq 1$ has been proposed.[4] This approach attempts to generalize the scaling (1), usually considered with b constant, to space-dependent rescaling $b = b(\vec{r}_\perp, r_{||})$, thereby assuming that the two-point functions still transform in a simple way. These transformations are constructed, starting from the conformal transformations $r_{||} \to (\alpha r_{||} + \beta)/(\gamma r_{||} + \delta)$ with $\alpha\delta - \beta\gamma = 1$, in such a way that the transformations in the 'spatial' coordinates $\vec{r}_\perp$ are consistent with the anisotropic scaling (1). Systems which are invariant under these transformations and whose correlators, generalizing (1), transform covariantly under them, are said to satisfy *local scale invariance* (LSI). It turns out that if $\theta = 2/N$, where N is a positive integer, $\Omega(v)$ satisfies the differential equation[4]

$$\alpha_1 \frac{\mathrm{d}^{N-1}\Omega(v)}{\mathrm{d}v^{N-1}} - v^2 \frac{\mathrm{d}\Omega(v)}{\mathrm{d}v} - \zeta v \Omega(v) = 0 \qquad (2)$$

where $\zeta = 2x/\theta$ and α_1 is a constant. Eq. (2) can be explictly solved[4] in terms of hypergeometric functions ${}_2F_{N-1}$ (conformal invariance is reproduced[4] for $N = 2$ and $N = 1$ gives the non-relativistic Schrödinger invariance[5]). Evidently, the above hypothesis of LSI in systems satisfying (1) is a strong one and relies on certain assumptions about the structure of the underlying field theory. In this letter, we shall test the idea of LSI by explicitly checking the resulting expressions for $\Omega(v)$ in a non-trivial spin system which satisfies the strongly anisotropic scaling (1).

While dynamical scaling (1) occurs in critical dynamics (then θ is referred to as dynamical exponent) or in true non-equilibrium phase transitions such as directed percolation, well-known examples of stongly anisotropic *equilibrium* criticality are the *Lifshitz points*[6] encountered in systems with competing interactions. At a Lifshitz point, a disordered, an uniformly ordered and a periodically ordered phase become indistinguishable.[6] The simplest model for these is the ANNNI (axial next-nearest neighbour Ising) model[7] which describes faithfully, among others, magnetic systems, alloys or uniaxially modulated ferroelectrics.[8–10] Recently, a large variety of new physical systems (ferroelectric liquid crystals,[11] uniaxial ferrolectrics,[12] block copolymers[13] or even quantum systems[14]) were shown to possess a Lifshitz point which has stimulated renewed interest in its properties. Furthermore, new field theory studies[15–18] have lead to more refined estimates (in the framework of an ϵ-expansion) of the critical exponents of the general m-fold Lifshitz points in d dimensions with a n-component order parameter.[15–17]

Here, we study the $3D$ ANNNI model, defined on a cubic lattice with periodic boundary conditions. The Hamiltonian is

$$\mathcal{H} = -J \sum_{xyz} s_{xyz} \left(s_{(x+1)yz} + s_{x(y+1)z} + s_{xy(z+1)} \right) + \kappa J \sum_{xyz} s_{xyz} s_{xy(z+2)} \qquad (3)$$

with $s_{xyz} = \pm 1$, whereas $J > 0$ and $\kappa > 0$ are coupling constants. In z-direction competition between ferromagnetic nearest neighbour and antiferromagnetic next-nearest neighbour couplings takes place, leading to a

rich phase diagram with a multitude of different phases, both commensurate and incommensurate to the underlying cubic lattice.[7] The anisotropy exponent $\theta = \nu_{||}/\nu_{\perp}$, where $\nu_{||}$ und $\nu_{\perp}$ are the exponents of the correlation lengths parallel and perpendicular to the z-axis. At the uniaxial Lifshitz point, a recent careful field-theoretical calculation[16] shows that $\theta = \frac{1}{2} - a\epsilon^2 + O(\epsilon^3)$ in a second-order ϵ-expansion (with $\epsilon = 4.5 - d$) where $a \simeq 0.0054$ for the $3D$ ANNNI model.

Our main purpose will be the numerical computation and thorough analysis of the critical spin-spin correlation function *at* the uniaxial Lifshitz point of the ANNNI model through a large-scale Monte Carlo simulation. The agreement between our numerical results and the analytic expression for $\Omega(v)$ derived from (2) presents evidence that local scale invariance, as formulated in Ref. 4, is realized as a new symmetry in strongly anisotropic equilibrium critical systems.

Such a study does require reliable and precise estimates of the critical exponents. However, published estimates of critical exponents obtained with different techniques spread considerably, see Table I. We therefore undertook large-scale Monte Carlo simulations to estimate the exponents reliably. Previous Monte Carlo studies[19] considered only small systems of (mostly) cubic shape. Here, we present calculations for large systems of anisotropic shape with $L \times L \times N$ spins, with $20 \leq L \leq 240$ and $10 \leq N \leq 100$, taking into account the special finite-size effects coming from the anisotropic scaling at the Lifshitz point.[21] This is the first study of the ANNNI model where the exponents α, β, and γ are computed independently.

As usual, the problems coming from critical slowing-down encountered when using local Monte Carlo dynamics, are alleviated by using non-local methods, such as the Wolff cluster algorithm.[22] For the Ising model with only a nearest neighbour coupling J, this algorithm may be described as follows: one chooses randomly a lattice site, the seed, and then builds up iteratively a cluster by including a lattice site j (with spin s_j), neighbour to a cluster site i (with spin s_i), with probability $p = \frac{1}{2}\left(1 + \mathrm{sign}\left(s_i s_j\right)\right)\left(1 - \exp\left[-2J/(k_B T)\right]\right)$. One ends up with a cluster of spins having all the same sign which is then flipped as a whole. This kind of same-sign clusters are obviously not adapted to our problem because of the competing interactions along the z-direction, see (3).

We therefore propose the following modified cluster algorithm. Starting with a randomly chosen seed, one again builds up iteratively a cluster. Consider a newly added cluster lattice site i with spin s_i. A lattice site j with spin s_j nearest neighbour to i is included with probability $p_{\mathrm{n}} = p$, whereas an *axial* next-nearest neighbour site k with spin s_k is included with probability $p_{\mathrm{a}} = \frac{1}{2}\left(1 - \mathrm{sign}\left(s_i s_k\right)\right)\left(1 - \exp\left[-2J\kappa/(k_B T)\right]\right)$. Thus, the final cluster, which will be flipped as a whole, contains spins of both signs. Ergodicity and detailed balance are proven as usual. This algorithm works extremely well in the ferromagnetic phase and in the vicinity of the Lifshitz point. Generalization to other systems with competing interactions is straightforward. For the computation of the spin-spin correlation function we adapt in a similar way a recently proposed very efficient algorithm using Wolff clusters.[24] This algorithm yields the infinite-system correlation functions at temperatures above T_c and largely reduces finite-size effects at the critical temperature as compared to a more traditional approach. These algorithms will be discussed in detail elsewhere.[23]

We now outline the determination of the critical exponents. The results are listed in Table I. As an example, Figure 1 shows the effective exponent

$$\beta_{\mathrm{eff}} = \frac{\mathrm{d}\ln m}{\mathrm{d}\ln t}, \tag{4}$$

where m denotes the magnetization and $t = 1 - T/T_c$. In the limit $t \to 0$ the effective exponent yields the critical exponent[25] β, provided finite-size effects can be neglected. The two sets of data in Figure 1 correspond to two different paths in the temperature-interaction space, both ending at the point ($\kappa = 0.270$, $T_c = 3.7475$), setting $J/k_B = 1$. For set (a) κ was fixed at 0.270, whereas for set (b) $\kappa = 0.270 + 1.6\,(1/T - 1/T_c)$. The corrections to scaling for set (b) are small compared to set (a), resulting in a plateau for $t \leq 0.06$, thus making a very precise estimation of β possible. Of course, finite-size effects have to be monitored carefully. As usual, we adjust the system size in order to circumvent finite-size dependences.[25,23] For the determination of the susceptibility and specific heat critical exponents γ and α, see Table I, data obtained at temperatures both below and above T_c were analysed. Our error bars take into account the sample averaging as well as the uncertainty in the location of the Lifshitz point. Based on our data, we locate the Lifshitz point at $\kappa = 0.270 \pm 0.004$, $T_c = 3.7475 \pm 0.0005$, thus confirming an estimation from a high temperature series expansion.[26]

The agreement of the independently estimated exponents α, β and γ with the scaling relation $\alpha + 2\beta + \gamma = 2$, up to $\approx 0.8\%$, illustrates the reliability of our data.

We are now ready to discuss the scaling of the spin-spin correlation function $C\left(\vec{r}_{\perp}, r_{||}\right) = \left\langle s_{\vec{r}_{\perp}, r_{||}}\, s_{\vec{0},0} \right\rangle$ and its scaling function $\Omega(v)$ as defined in (1). In $(d_{\perp}+1)$ dimensions, one has $\zeta = 2(d_{\perp} + \theta)/\theta(2 + \gamma/\beta)$. For the $3D$ ANNNI model, $\zeta = 1.30 \pm 0.05$, where the error follows from the errors in the values of the critical exponents. In Figure 2 we show selected data for the function

$$\Phi(u) = u^{-\zeta}\,\Omega(1/u) \tag{5}$$

with $u = \sqrt{r_{\perp}}/r_{||}$, as computed by Monte Carlo simulations of a system with $200 \times 200 \times 100$ spins (assuming[27] $\theta = 1/2$). This permits a nice visual test of the data collapse and establishes scaling.

The small deviations (of order $\approx 2\%$) from the value $\theta = 1/2$ obtained in recent field-theoretical calculations[16] are not yet distinguishable[27] from the purely numerical errors in our data and the exponents derived from them.

Therefore, for our purposes, namely the test of LSI, it is enough to set $\theta = 2/N = 1/2$, leading to $N = 4$ in the differential equation (2). In addition, the scaling form (1) implies the boundary condition $\Omega(v) \sim v^{-\zeta}$ for $v \to \infty$. For $N = 4$, there are two independent solutions of eq. (2) satisfying this boundary condition[3,4] and the scaling function becomes

$$\Omega(v) = b_0 F_0(v/(4\alpha_1)^{1/4}) + b_1 v F_1(v/(4\alpha_1)^{1/4}) \qquad (6)$$

where[4]

$$F_0(x) = \frac{\Gamma(3/4)}{\Gamma(\zeta/4)} \sum_{n=0}^{\infty} \frac{\Gamma(n/2+\zeta/4)}{n!\Gamma(n/2+3/4)} \left(-x^2\right)^n \qquad (7)$$

$$F_1(x) = \frac{\Gamma(3/2)}{\Gamma(\frac{1}{4}(\zeta+1))} \sum_{n=0}^{\infty} \frac{\Gamma((n+1+\zeta)/4) s(n)}{\Gamma(n/4+1)\Gamma(\frac{1}{2}(n+3))} (-x)^n$$

and $s(n) = \frac{1}{\sqrt{2}}(\cos\frac{n\pi}{4} + \sin\frac{n\pi}{4})\cos\frac{n\pi}{4}$. Here α_1 is the constant occuring in (2) and $b_{0,1}$ are free parameters. Since b_0 and α_1 are merely scale factors, the functional form of the scaling functions $\Omega(v)$ and $\Phi(u) = u^{-\zeta}\,\Omega(1/u)$ depends on the single *universal* parameter $p := \alpha_1^{1/4} b_1/b_0$.

To see this, consider the moments $M(n) := \int_0^\infty du\, u^n\, \Phi(u)$. For $\theta = 1/2$ and taking into account (6), it follows[28] that in the scaling region the moment ratios

$$J(\{m_i\};\{n_j\}) := \prod_{i=1}^{k} M(m_i) \Big/ \prod_{j=1}^{k} M(n_j) \qquad (8)$$

with $k \geq 2$ and $\sum_i m_i = \sum_j n_j$ are independent of b_0 and α_1 and only depend on the functional form of $\Phi(u)$ as parametrized by p. Our Monte Carlo data for the spin-spin correlator will be consistent with LSI if the values of p determined from several different ratios J coincide.

As we are not able to compute numerically the function $\Phi(u)$ for values of u below $u_0 \approx 0.22$ a direct analysis along the lines just sketched is not possible. Instead we have to consider the moments $\widetilde{M}(n) := \int_{u_0}^\infty du\, u^n\, \Phi(u\,\alpha_1^{1/4}) = \alpha_1^{-(n+1)/4} \int_{w_0}^\infty dw\, w^n\, \Phi(w)$ with $w_0 = u_0\,\alpha_1^{1/4}$. The moment ratios $\widetilde{J}(\{m_i\};\{n_j\})$ (defined in complete analogy with (8)) then depend on the scale factor $\alpha_1^{1/4}$ through w_0. The parameters α_1 and p are determined from the following scheme. Choosing a suitable starting value for α_1 we compute an approximative value for p by comparing the values of the moment ratios $\widetilde{J}$ (obtained from the full data set for $\Phi(u)$ as shown in the inset of Figure 2) with the p-dependent expressions coming from integrating the $\widetilde{M}(n)$ using the analytic form (6,7). An improved value for α_1 is then derived by comparing the values $\widetilde{M}(m)/\widetilde{M}(n)$ for arbitrary m and n obtained (i) from our numerical data and (ii) from the analytical expressions after inserting the value of p. The final values of α_1 are obtained by averaging over five different pairs (m,n).

The values of p and α_1 determined from several distinct moment ratios are collected in Table II. We obtain the mean values $p = -0.11(1)$ and $\alpha_1 = 33.2(8)$. The consistency of the different determinations of the two parameters provides clear evidence in favour of the applicability of the hypothesis of local scale invariance to the Lifshitz point of the ANNNI model.

Finally, $b_0 \approx 0.41$ is obtained by adjusting the scale of Φ. Inserting these values into the analytical expression yields for Φ the full curve shown in the inset of Figure 2. The agreement between our MC data and the theoretical result is remarkable.

Local scale invariance had been confirmed before at the Lifshitz point of the ANNNS model. In that exactly solvable model, the Ising model spins in (3) are replaced by spherical model spins $s_{xyz} \in \mathbb{R}$ together with the usual spherical constraint.[7] At the Lifshitz point, one has $\theta = 1/2$ and the exactly known spin-spin correlator[29] agrees with the scaling form (6) for $b_1 = 0$.[4] Our finding that LSI also appears to hold for the ANNNI model suggests that the domain of validity of LSI should extend beyond the context of free field theory which underlies the ANNNS model. It appears plausible that LSI will also hold true for the Lifshitz points of the ANNNXY, ANNNH,...models[7] which are intermediate between the ANNNI and the ANNNS model. Since the number of dimensions $d_\perp$ merely enters as a parameter, local scale invariance could also be tested along the lines of an ϵ-expansion.[16] Finally, the consistency of other correlators (e.g. energy-energy) with LSI should be tested. We plan to come back to this elsewhere. It would be tempting to see whether the powerful techniques of $2D$ conformal invariance[2] might be extended to the situation of anisotropic scaling realized at Lifshitz points. This would lead to numerous physical applications[8–14] and is under investigation.

In conclusion, the precise localisation of the $3D$ ANNNI model Lifshitz point and improved estimates of its critical exponents allowed for the first time to determine reliably the scaling of the spin-spin correlator. Its functional form was found to agree with the prediction of local scale invariance. The confirmation of the applicability of local scale invariance to this situation suggests a new symmetry principle for the description of equilibrium systems with anisotropic scaling, especially for systems with competing interactions at their Lifshitz points.

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[1] J.L. Cardy, *Scaling and Renormalization in Statistical Mechanics* (Cambridge University Press, Cambridge, 1996).

[2] A.A. Belavin, A.M. Polyakov, and A.B. Zamolodchikov, Nucl. Phys. **B241**, 333 (1984).
[3] M. Henkel, *Conformal Invariance and Critical Phenomena* (Springer, Heidelberg, 1999).
[4] M. Henkel, Phys. Rev. Lett. **78**, 1940 (1997).
[5] M. Henkel, J. Stat. Phys. **75**, 1023 (1993); T. Mehen, I.W. Stewart and M.B. Wise, Phys. Lett. **B474**, 145 (2000).
[6] R.M. Hornreich, M. Luban, and S. Shtrikman, Phys. Rev. Lett. **35**, 1678 (1975).
[7] W. Selke, in *Phase Transitions and Critical Phenomena*, Vol.15, edited by C. Domb and J.L. Lebowitz (Academic Press, New York, 1992).
[8] W. Selke, Phys. Rep. **170**, 213 (1988).
[9] J.M. Yeomans, Solid State Physics **41**, 151 (1988).
[10] B. Neubert, M. Pleimling, and R. Siems, Ferroelectrics **208-209**, 141 (1998).
[11] M. Škarabot, R. Blinc, I. Muševič, A. Rastegar, and Th. Rasing, Phys. Rev. **E61**, 3961 (2000).
[12] Y. M. Vysochanskii and V. U. Slivka, Usp. Fiz. Nauk **162**, 139 (1992).
[13] F.S. Bates, W. Maurer, T.P. Lodge, M.F. Schulz, M.W. Matsen, K. Almdal, and K. Mortensen, Phys. Rev. Lett. **75**, 4429 (1995).
[14] A. Schröder, G. Aeppli, E. Bucher, R. Ramazashvili, and P. Coleman, Phys. Rev. Lett. **80**, 5623 (1998).
[15] C. Mergulhão, Jr. and C.E.I. Carneiro, Phys. Rev. **B58**, 6047 (1998) and **B59**, 13954 (1999).
[16] H.W. Diehl and M. Shpot, Phys. Rev. **B62**, 12338 (2000).
[17] H.W. Diehl and M. Shpot, private communication.
[18] M.M. Leite, Phys. Rev. **B61**, 14691 (2000).
[19] K. Kaski and W. Selke, Phys. Rev. **B31**, 3128 (1985).
[20] Z. Mo and M. Ferer, Phys. Rev. **B43**, 10890 (1991).
[21] K. Binder and J.-S. Wang, J. Stat. Phys. **55**, 87 (1989); K.-t. Leung, Phys. Rev. Lett. **66**, 453 (1991).
[22] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).
[23] M. Pleimling and M. Henkel, unpublished.
[24] H. G. Evertz and W. v. d. Linden, `cond-mat/0008072`.
[25] M. Pleimling and W. Selke, Eur. Phys. J. **B1**, 385 (1998).
[26] J. Oitmaa, J. Phys. A: Math. Gen. **18**, 365 (1985).
[27] Using $\theta = 0.488$ as suggested in Ref. 16 does not lead to a perceptible modification of the scaling plot.
[28] J. Benzoni, J. Phys. A: Math. Gen. **17**, 2651 (1984).
[29] L. Frachebourg and M. Henkel, Physica **A195**, 577 (1993).

TABLE I. Critical exponents at the Lifshitz point of the $3D$ ANNNI model, as obtained from Monte Carlo simulations (MC), high-temperature series expansion (HT) and renormalized field theory (FT). The numbers in brackets give the estimated error in the last digit(s).

	α	β	γ	$(2-\alpha)/\gamma$	β/γ
MC [19]		0.19(2)	1.40(6)		0.14(2)
HT [20]	0.20(15)		1.6(1)	1.1(2)	
FT [16]				1.27	0.134
FT [17]	0.160	0.220	1.399	1.315	0.157
MC	0.18(2)	0.238(5)	1.36(3)	1.34(5)	0.175(8)

TABLE II. Values of the parameters p and α_1 computed from different moment ratios $\widetilde{J}(\{m_i\};\{n_j\})$, see text.

$\{m_i\}$	$\{n_j\}$	p	α_1
$\{0,-0.5\}$	$\{-0.25,-0.25\}$	-0.102	32.7
$\{-0.25,-0.75\}$	$\{-0.5,-0.5\}$	-0.125	34.0
$\{0.2,-0.9\}$	$\{0,-0.7\}$	-0.100	32.8
$\{0.2,-0.6,-0.8\}$	$\{-0.3,-0.4,-0.5\}$	-0.102	32.8
$\{-0.1,-0.6,-0.7\}$	$\{-0.4,-0.5,-0.5\}$	-0.117	33.5

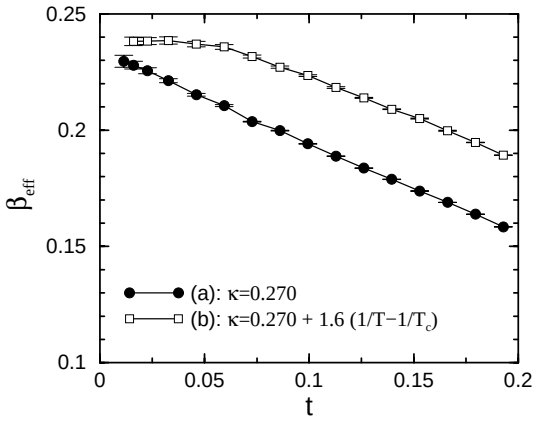

FIG. 1. Effective exponent $\beta_{\rm eff}$ versus t for two different trajectories in the (T,κ) space, see text. Error bars include the uncertainty in T_c: $T_c(\kappa = 0.270) = 3.7475 \pm 0.0005$.

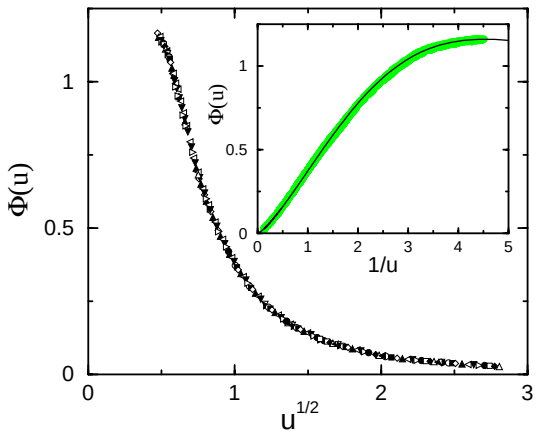

FIG. 2. Scaling funtion $\Phi(u)$ (see text) versus $u^{1/2} = (\sqrt{r_\perp}/r_\parallel)^{1/2}$ for $\kappa = 0.270$ and $T = 3.7475$. Selected Monte Carlo data for a system of $200 \times 200 \times 100$ spins are shown.[27] The different symbols correspond to the values of $r_\perp$. Inset: comparison of the full data set of $1.7 \cdot 10^4$ points for the scaling function $\Phi(u)$ (gray points) with the analytical prediction eqs. (6,7) following from the assumption of LSI, with $p = -0.11$, $\alpha_1 = 33.2$ and $b_0 = 0.41$ (full curve).